Intellegens machine learning for materials design
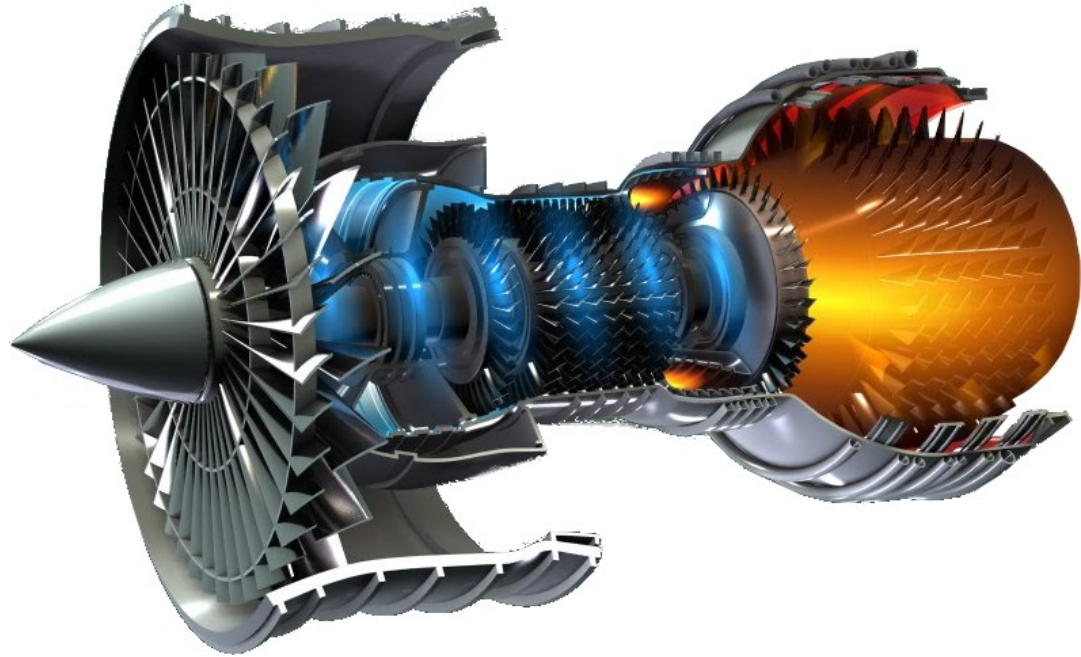
Technology developed at **University of Cambridge** with three features
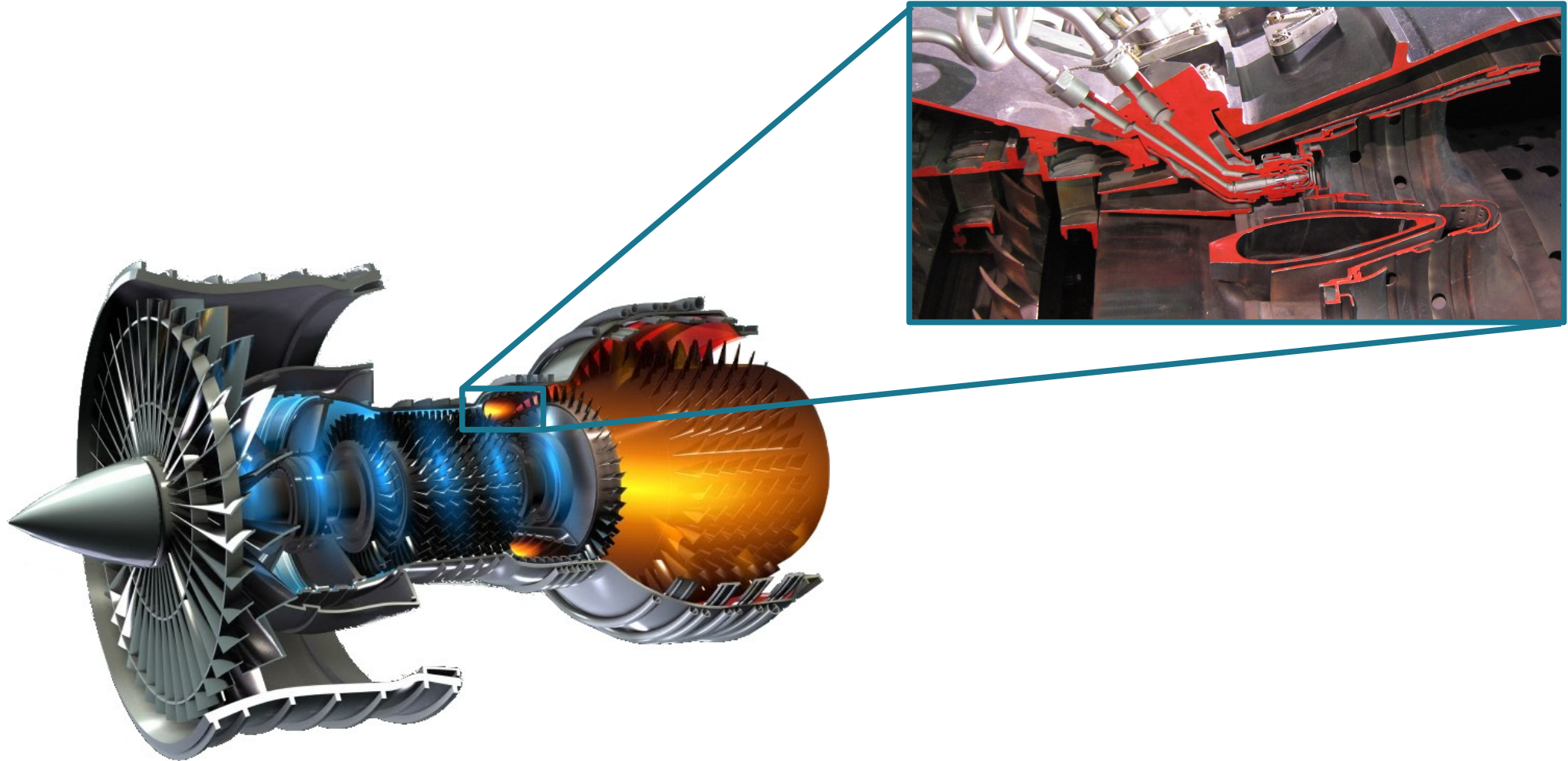
Design for **multiple target properties**

Merge simulations, physical laws, and experimental data to exploit all available information

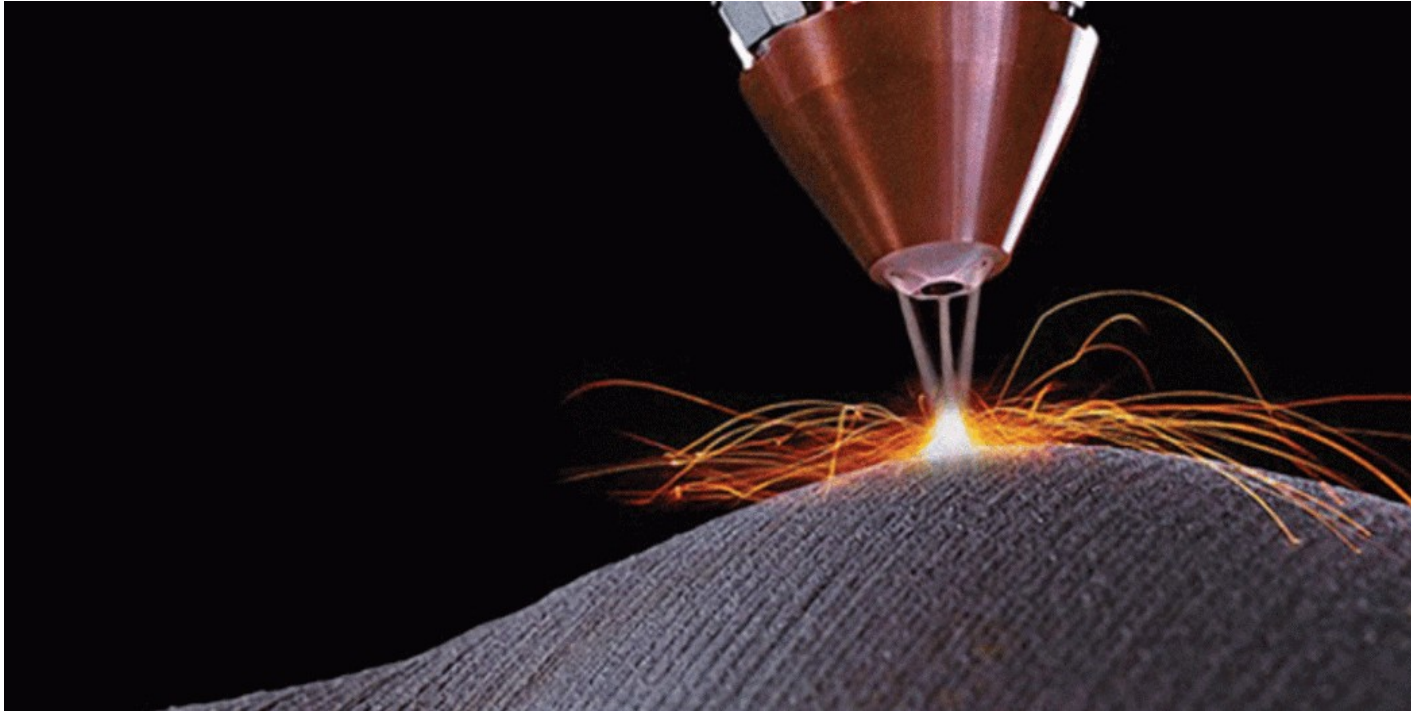Probabilistic algorithm finds material **most likely** to succeed

Schematic of a jet engine
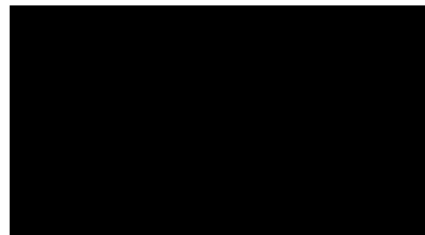
Combustor in a jet engine

Direct laser deposition requires new alloys

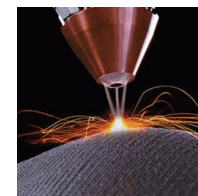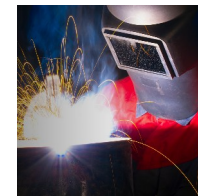# Black box machine learning for materials design

Composition

Properties

Defects

Fatigue

Welding

Train the machine learning
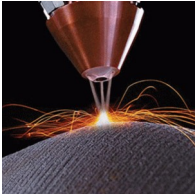
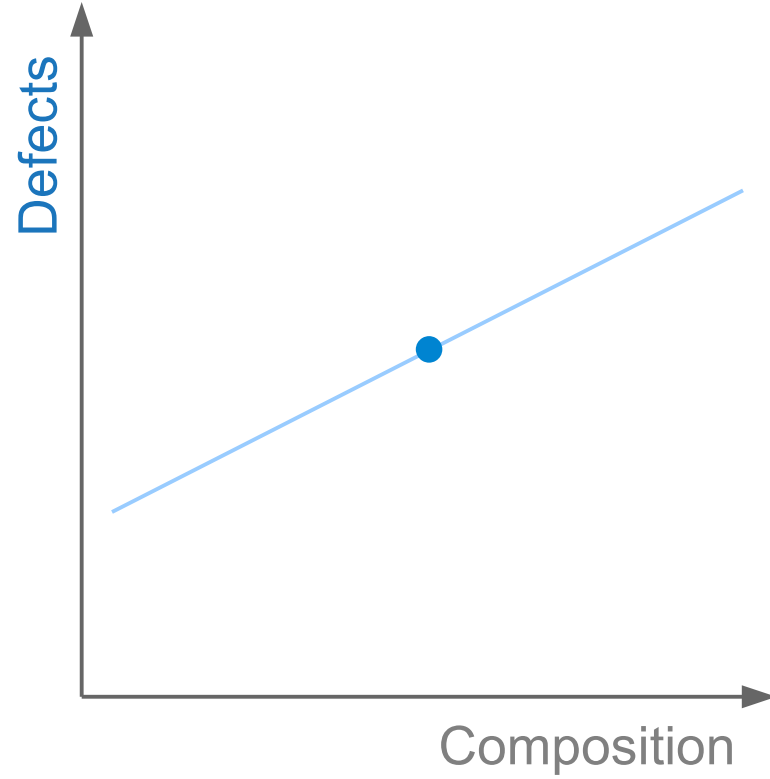# Machine learning model for materials design
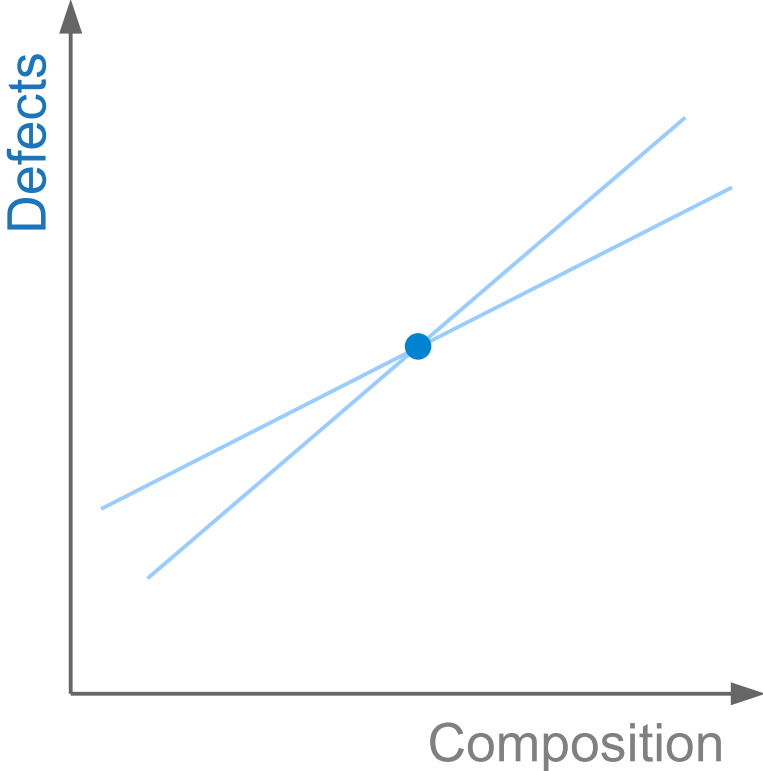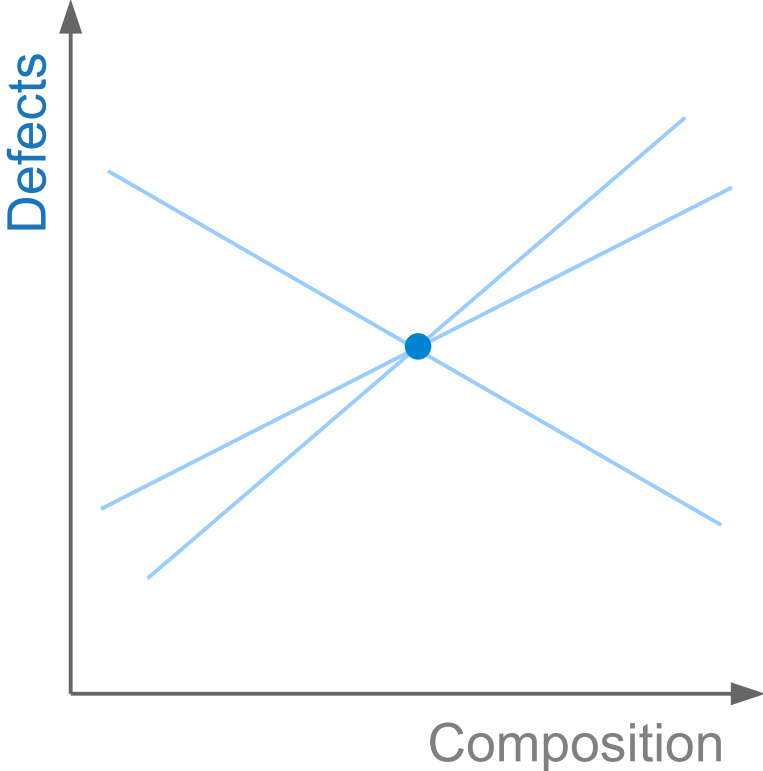
Composition

Properties
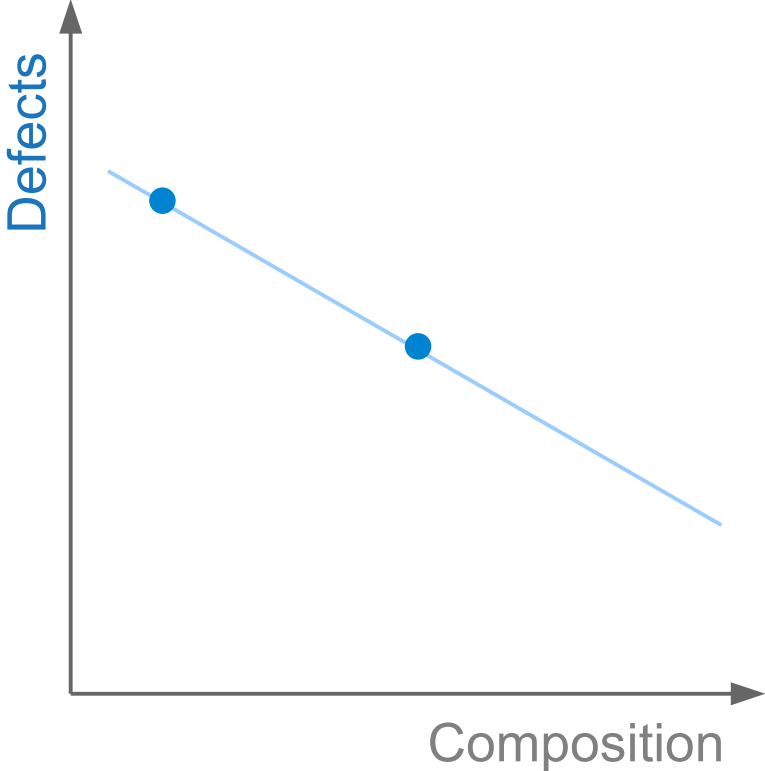
Defects

Fatigue

Welding

One point cannot define a straight line

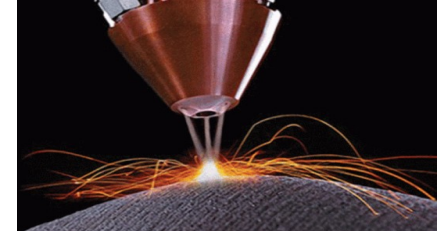# One point cannot define a straight line

One point cannot define a straight line

Need at least two points to define a straight line
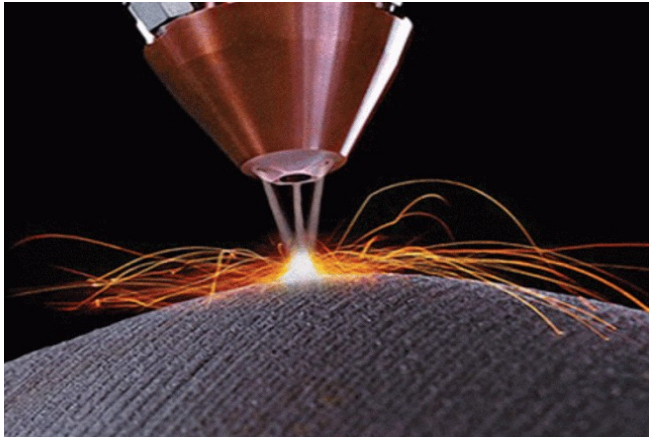
Data required for a defects model

Composition and heat treatment space 30 dimensions

Requires 31 points to fit a hyperplane

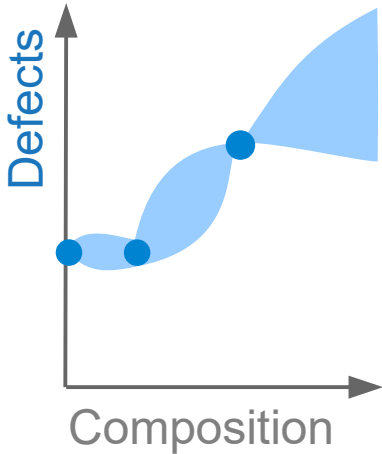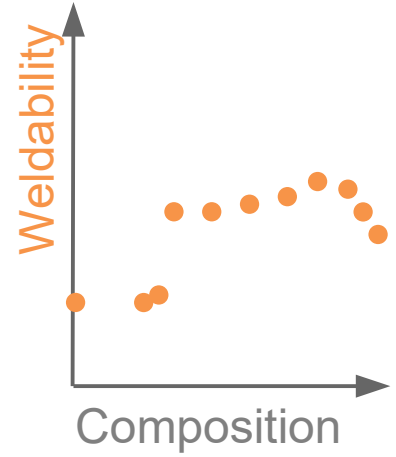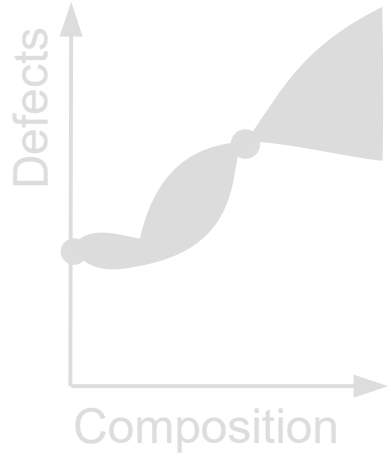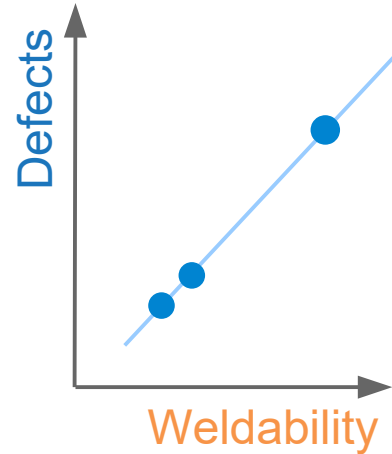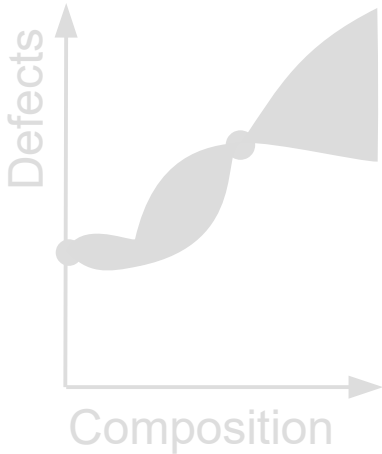Just 8 data points available

Neural networks for materials design
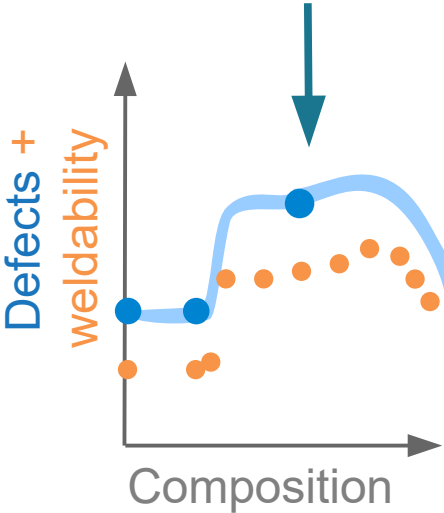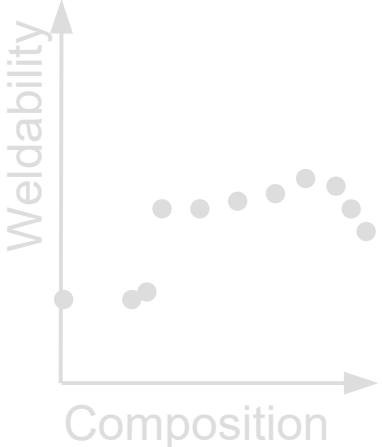

Laser

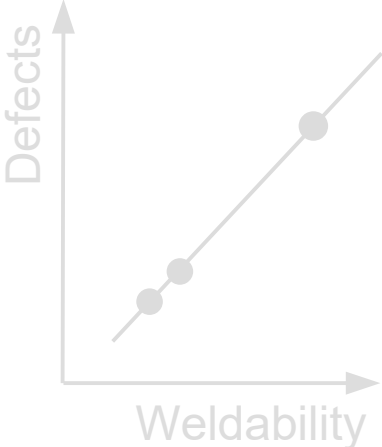Electricity

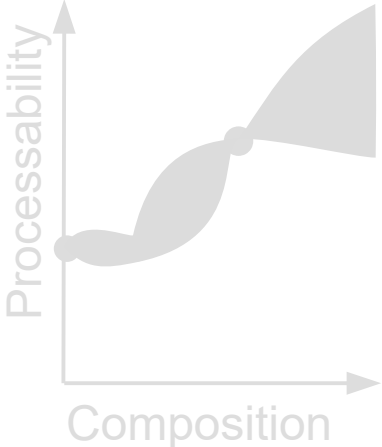# Insufficient data for processability

Welding is analogous to direct laser deposition
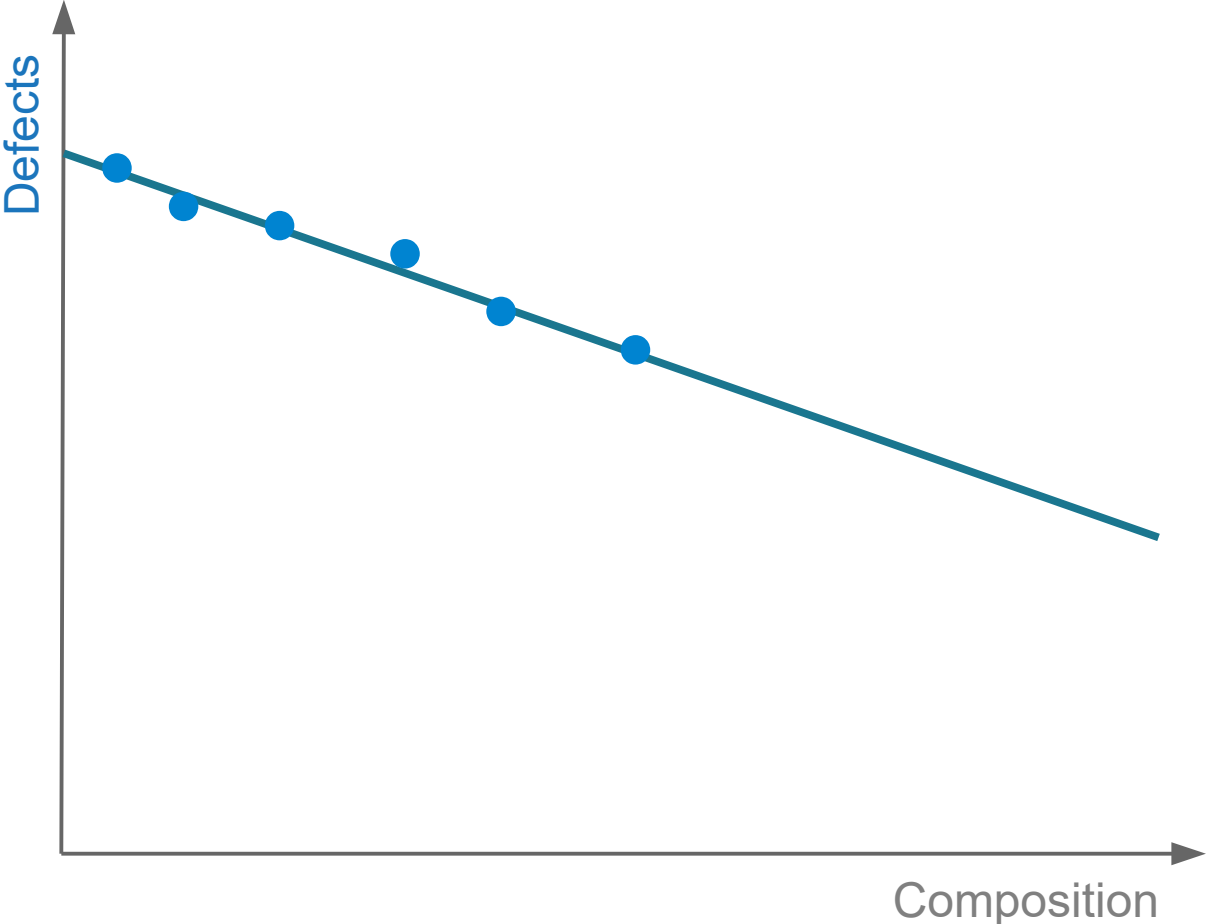
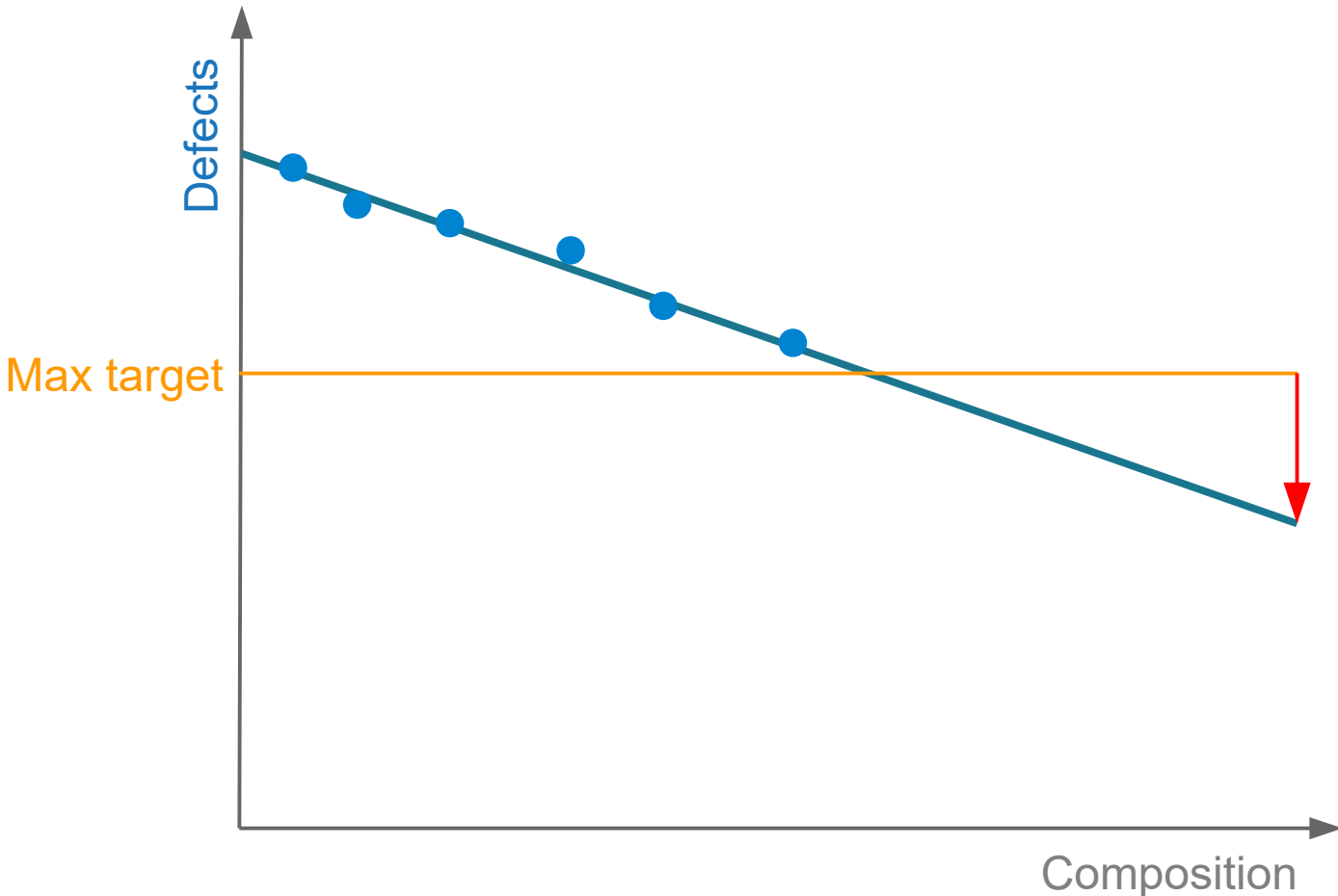# Simple processability-welding relationship

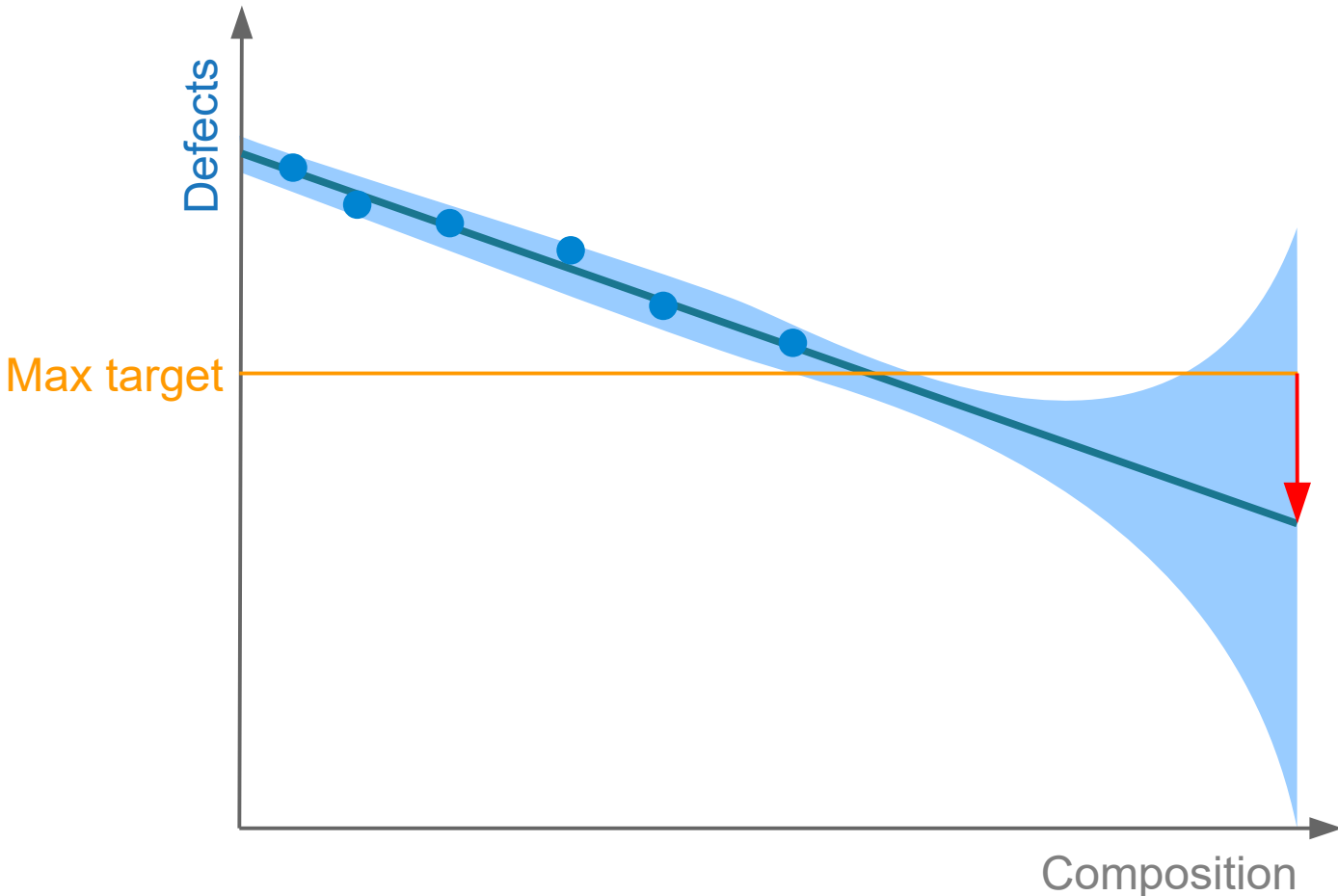# Merging properties with the neural network

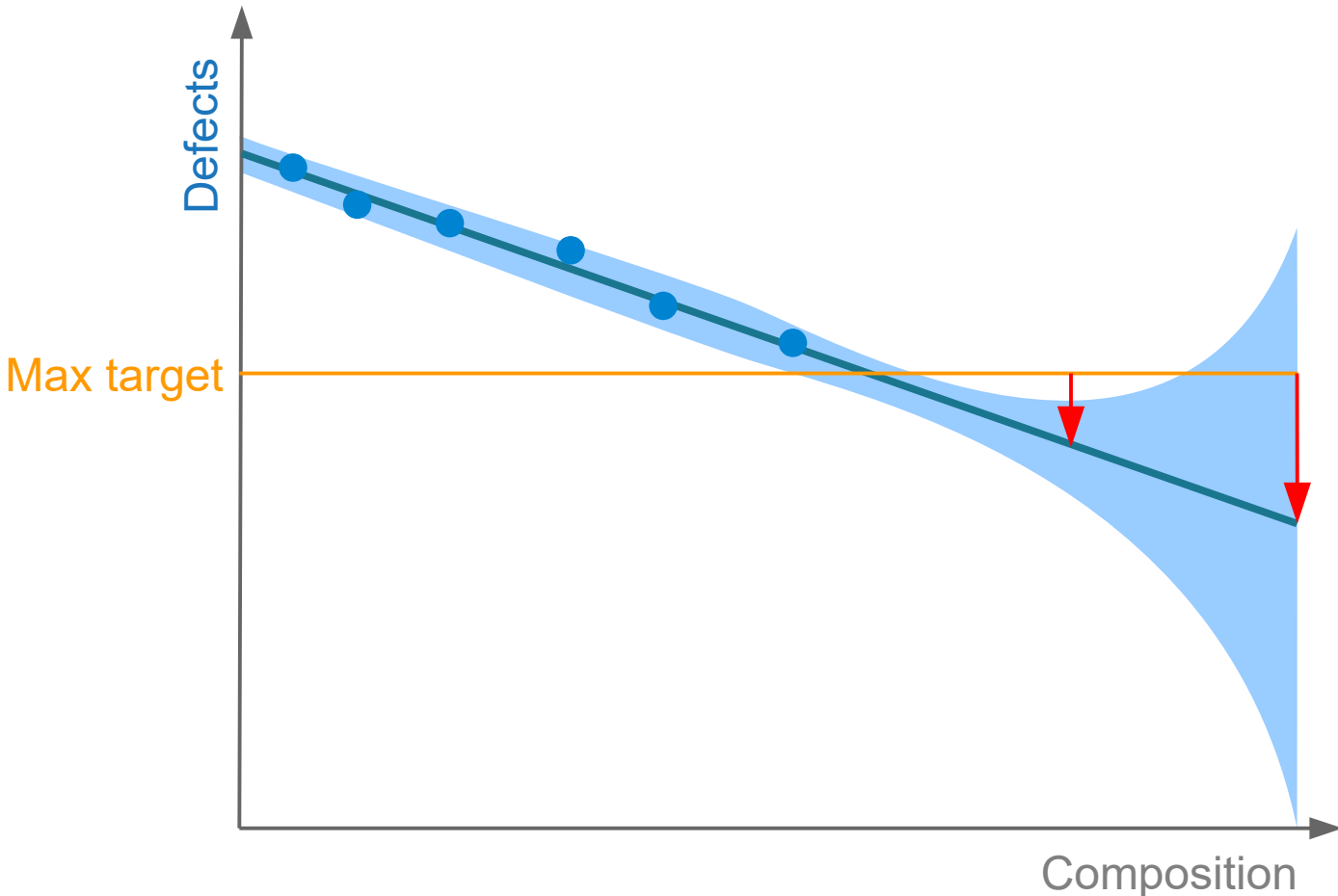# Simple straight line fit to data
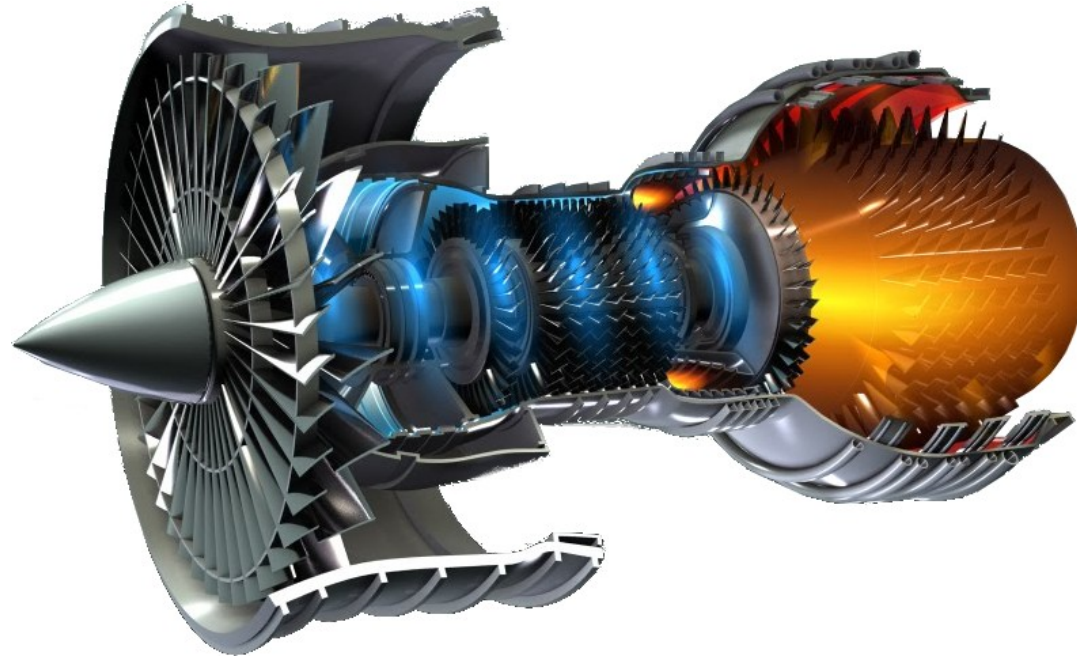
Usually design to exceed target

Design the material most likely to succeed

Design the material most likely to succeed

Schematic of a jet engine

Target properties

Elemental cost < 25 \$kg^{-1}

Density < 8500 kgm^{-3}

γ' content < 25 wt%

Oxidation resistance < 0.3 mgcm^{-2}

Defects $< 0.15\%$ defects

Phase stability > 99.0 wt%

γ' solvus > 1000°C

Thermal resistance > 0.04 KΩ^{-1}m^{-3}

Yield stress at 900°C > 200 MPa

Tensile strength at 900°C > 300 MPa

Tensile elongation at 700°C $> 8\%$

1000hr stress rupture at 800°C > 100 MPa

Fatigue life at 500 MPa, 700°C $> 10^5$ cycles
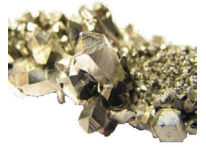
Composition

Cr 19%
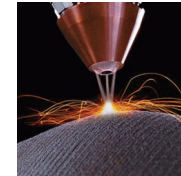
Co 4%

Mo 4.9%

W 1.2%

Zr 0.05%

Nb 3%

Al 2.9%

C 0.04%

B 0.01%

Ni

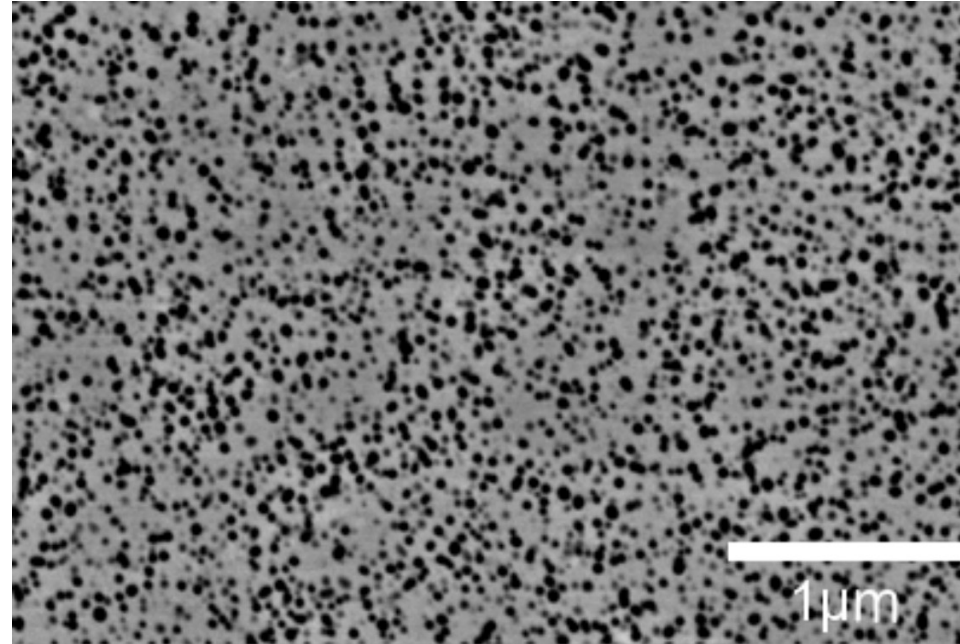Expose 0.8

T_{HT} 1300ºC

Microstructure

Testing the defect density

Testing the oxidation resistance

More materials designed

Nickel and molybdenum

Steel for welding

Experiment and DFT for batteries

Application to industrial chemicals

Ink formulations

Lubricants

Small molecule drug design

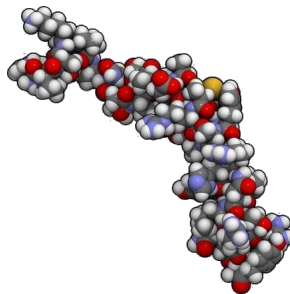# Summary

Merge different experimental quantities and computer simulations into a **holistic** design tool
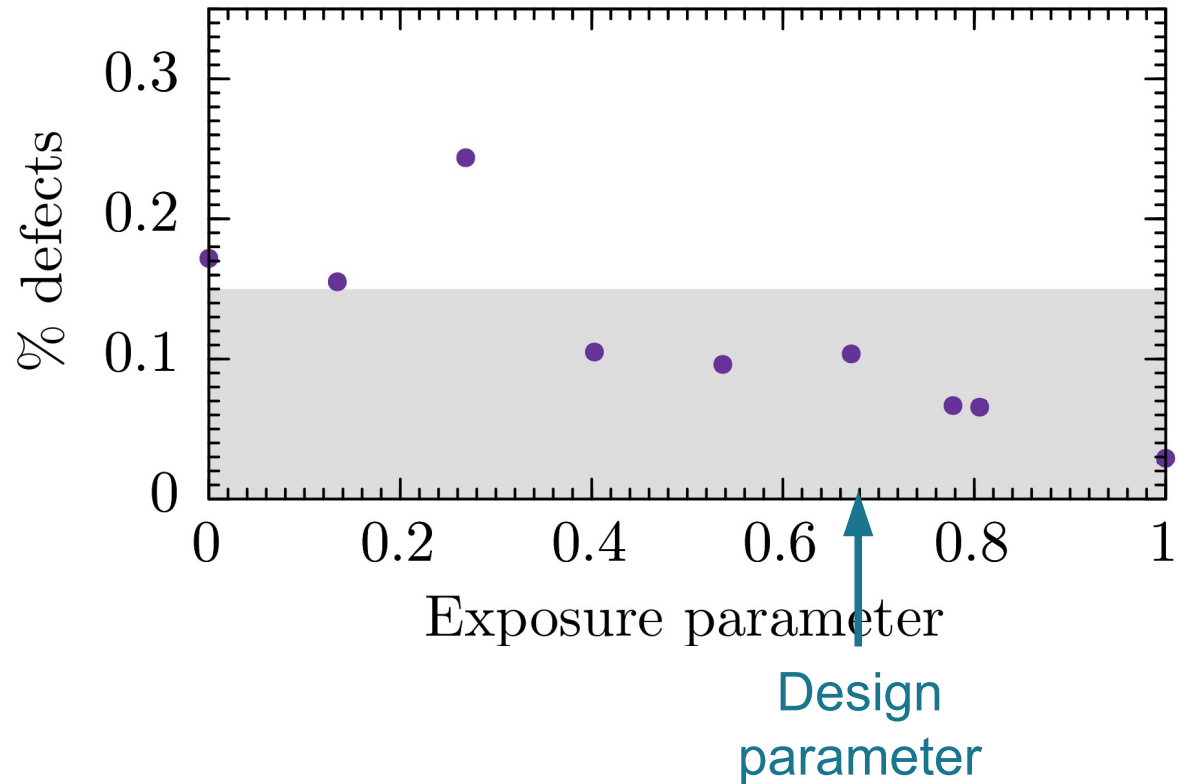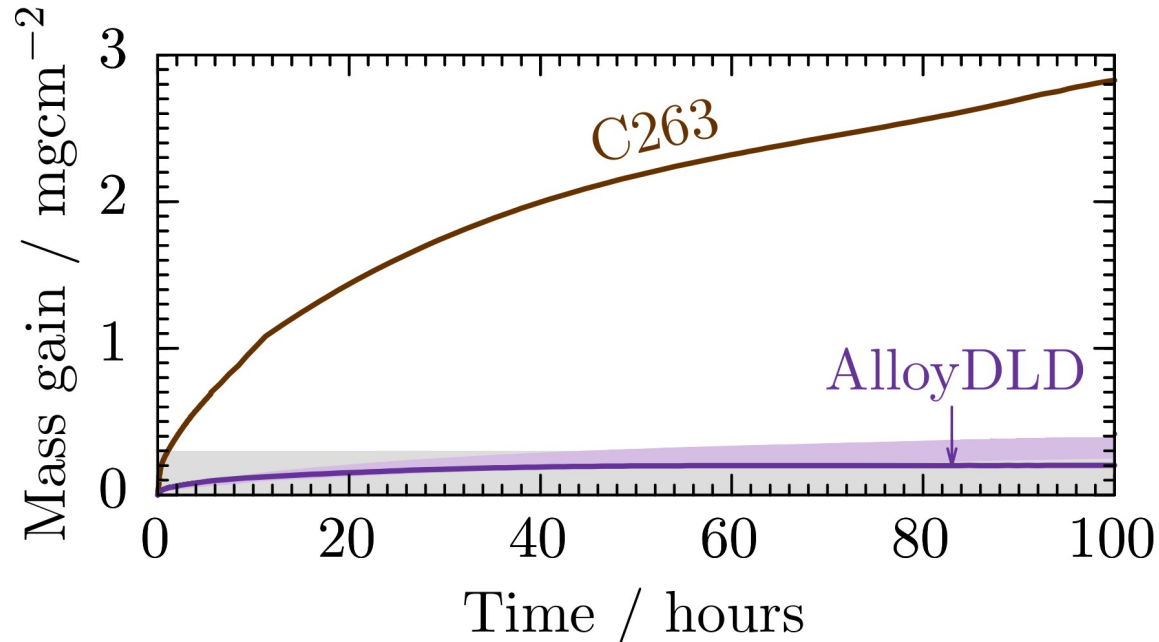
Designed and experimentally verified alloy for **direct laser deposition**

Designed and many other experimentally verified **materials** and **drugs**